Isospin-symmetry-breaking corrections to superallowed Fermi β decay: Formalism and schematic models

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We study the formalism to include isospin-symmetry-breaking corrections when extracting the up-down Cabibbo-Kobayashi-Maskawa matrix element from superallowed $0^+ \to 0^+$ nuclear β decay. We show that there are no first order isospin-symmetry-breaking corrections to the relevant nuclear matrix elements. We find corrections to the treatment of Towner and Hardy, and assess these using schematic models of increasing complexity.

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I. INTRODUCTION

Superallowed Fermi β decay provides the most stringent test of the conserved-vector-current (CVC) hypothesis, the most precise value for the up-down Cabibbo-Kobayashi-Maskawa (CKM) matrix element V_{ud}, and the best limit on the presence of scalar interactions. With the confirmation of CVC, V_{ud} can be extracted with great precision to test the Standard Model [1, 2, 3]. For this, one needs to evaluate $\sim 1\%$ theoretical corrections that arise due to nucleus-dependent isospin-symmetry-breaking (ISB) effects between the parent and daughter states, and due to radiative effects [4, 5]. These corrections are small, but significant, and their associated theoretical errors at present dominate the uncertainty of V_{ud} because of the very high precision reached experimentally [6].

In the 2005 survey of Hardy and Towner [1], the results for the set of superallowed $0^+ \to 0^+$ transitions were statistically consistent, after including these theoretical corrections. However, Penning-trap measurements of the transition energy for ^{46}V [7, 8] moved this case to more than two standard deviations away from the 2005 survey. This lead Towner and Hardy (TH) [6] to reexamine their treatment of ISB corrections and to include the contribution from core orbitals. The latter were found to be especially important for ^{46}V and this anomaly disappeared.

In this paper, we study the formalism to include ISB corrections, and contrast the TH treatment to exact results. Before proceeding, we review the necessary theoretical background, following the discussion in TH [6].

Superallowed $0^+ \to 0^+$ Fermi β decay depends only on the vector part of weak interactions, and with CVC, the decay transition "ft value" should be independent of the nucleus:

$$ft = \frac{2\pi^3 \hbar^7 \ln 2}{|M_F|^2 \, G_V^2 m_e^5 c^4} = \text{const.}\,, \tag{1}$$

where G_V is the vector coupling constant and M_F is the Fermi matrix element. CVC depends on the assumption of isospin symmetry, which is not exact in nuclei, but broken by electromagnetic and quark mass effects. As a result, M_F is reduced from its symmetry value of $M_0 = \sqrt{2}$ for $T = 1$ parent and daughter states. Following TH, we introduce the ISB corrections δ_C to the Fermi matrix element by

$$|M_F|^2 = |M_0|^2 \, (1 - \delta_C)\,. \tag{2}$$

In addition, there are radiative corrections to Eq. (1), but we focus on δ_C here. These isospin corrections are $\sim 1\%$, but must be calculated with a theoretical uncertainty of 10%, to guarantee a desired accuracy of 0.1%. This presents a challenge for nuclear theory.

Hardy and Towner have shown [1, 6] that the calculated corrections eliminate much of the considerable scatter present in the uncorrected ft values, and the statistical consistency among the corrected values is evidence that the corrections have been reasonably computed. However, the importance of precisely testing the Standard Model stimulates us to undertake a reevaluation. With this, we wish to start and stimulate further efforts to systematically improve ISB corrections, based on an accurate understanding of ISB in nuclear forces [9, 10].

This paper is organized as follows. In Sect. II, we show that TH do not use the isospin operator to calculate δ_C (as mandated by the Standard Model). To examine potential consequences of this, we review the TH treatment in Sect. III. A complete formalism is presented in Sect. IV, where we show that there are no first order ISB corrections to the relevant nuclear matrix elements, which is also true for the work of TH. In Sect. V, we compare the TH treatment to exact model results of increasing complexity, which can guide future improvements. We conclude in Sect. VI.

II. TOWNER AND HARDY APPROACH TO ISB CORRECTIONS

In nuclei, the matrix elements of weak vector interactions are not modified by nuclear forces, except for cor-

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rections due to ISB effects. Therefore, one has to evaluate the contributions from electromagnetic and charge-dependent strong interactions to the Fermi matrix element $M_F = \langle f|\tau_+|i\rangle$ between the initial and final states for superallowed β decay, $|i\rangle$ and $|f\rangle$, respectively. Here τ_+ is the isospin raising operator.

Towner and Hardy [6] use a second quantization formulation to write the Fermi matrix element as

$$M_F = \sum_{\alpha,\beta} \langle f|a^\dagger_\alpha a_\beta|i\rangle \langle \alpha|\tau_+|\beta\rangle \,, \tag{3}$$

where $a^\dagger_\alpha$ creates a neutron in state α and a_β annihilates a proton in state β. Thus, the label α is used to denote neutron creation and annihilation operators, while β is used for those of the proton. This notation is different from the standard notation [11], in which b_α is used to denote proton annihilation operators.

The single-particle matrix element $\langle \alpha|\tau_+|\beta\rangle$ is assumed to be given by the expression

$$\langle \alpha|\tau_+|\beta\rangle = \delta_{\alpha,\beta} \int_0^\infty R^n_\alpha(r)\, R^p_\beta(r)\, r^2 dr \equiv \delta_{\alpha,\beta}\, r_\alpha \,, \tag{4}$$

where $R^n_\alpha(r)$ and $R^p_\beta(r)$ are the neutron and proton radial wave functions, respectively. The problem is that the correct superallowed beta decay operator in the Standard Model is the plus component of the isospin operator. The operator in Eq. (3) is not the isospin operator, because the states $|\alpha\rangle$ and $|\beta\rangle$ are not the same. Instead, τ_+ of Eq. (3) is the plus component of the W-spin operator of MacDonald [12], which is reviewed in Ref. [11]. In addition, Eq. (4) assumes that the radial quantum numbers of the states α and β must be the same. This need not be so. As a result, the Standard Model isospin commutation relations maintained in the W-spin formalism are lost.

To obtain the commutation relations, we observe that Eqs. (3) and (4) correspond to the second-quantized isospin operators

$$\tau_+ \;=\; \sum_{\alpha,\beta} \delta_{\alpha,\beta}\, r_\alpha\, a^\dagger_\alpha a_\beta \,, \tag{5}$$

$$\tau_- \;=\; \tau^\dagger_+ = \sum_{\alpha,\beta} \delta_{\alpha,\beta}\, r^*_\alpha\, a^\dagger_\beta a_\alpha \,, \tag{6}$$

so that

$$[\tau_+, \tau_-] = \sum_\alpha |r_\alpha|^2\, a^\dagger_\alpha a_\alpha - \sum_\beta |r_\beta|^2\, a^\dagger_\beta a_\beta \neq \tau_0 \,. \tag{7}$$

The Standard Model isospin commutation relations are violated if one uses the isospin operators of TH.

This formal problem motivates us to reevaluate the treatment of ISB corrections, and to study whether there are potential corrections to the extraction of V_{ud}. To this end, we review the details of the TH procedure for δ_C. Although Eqs. (3) and (4) are not formally correct, they do account for the important correction: the effects of the Coulomb interaction on the radial wave functions.

III. TH TREATMENT OF δ_C

Towner and Hardy [6] proceed by introducing into Eq. (3) a complete set of states for the $(A-1)$-particle system, $|\pi\rangle$, which leads to

$$M_F = \sum_{\alpha,\pi} \langle f|a^\dagger_\alpha|\pi\rangle \langle \pi|a_\alpha|i\rangle\, r^\pi_\alpha \,. \tag{8}$$

The TH model thus allows for a dependence of the radial integrals on the intermediate state π.

If isospin were an exact symmetry, the matrix elements of the creation and annihilation operators would be related by hermiticity, $\langle \pi|a_\alpha|i\rangle = \langle f|a^\dagger_\alpha|\pi\rangle^*$, and all radial integrals would be unity. Hence the symmetry-limit matrix element in this model is given by

$$M_0 = \sum_{\alpha,\pi} |\langle f|a^\dagger_\alpha|\pi\rangle|^2 \,. \tag{9}$$

Towner and Hardy divide the contributions from ISB into two terms. First, the hermiticity of the matrix elements of a_α and $a^\dagger_\alpha$ will be broken, and second, the radial integrals will differ from unity. Assuming both effects are small, TH calculate the resulting ISB corrections as [6]

$$\delta_C = \delta_{C1} + \delta_{C2} \,, \tag{10}$$

where in evaluating δ_{C1} all radial integrals are set to unity but the matrix elements are not assumed to be related by hermiticity, and in evaluating δ_{C2} it is assumed that $\langle \pi|a_\alpha|i\rangle = \langle f|a^\dagger_\alpha|\pi\rangle^*$ but $r^\pi_\alpha \neq 1$. We will study whether this is a useful representation of δ_C. However, we emphasize that the separation into δ_{C1} and δ_{C2} is a model-dependent concept, inspired by the shell model [4]. For example, this division is clearly model dependent when M_F is obtained from ab-initio calculations of the initial and final states, $|i\rangle$ and $|f\rangle$. In addition, we demonstrate below that this is not possible rigorously for schematic models.

A. Radial overlap correction δ_{C2}

Towner and Hardy find that the radial correction, δ_{C2}, is the larger of their two model corrections [4, 5, 6]. The Fermi matrix element relevant for δ_{C2} is given by

$$\begin{aligned} M_F \;&=\; \sum_{\alpha,\pi} |\langle f|a^\dagger_\alpha|\pi\rangle|^2\, r^\pi_\alpha \,, \\ &=\; M_0 \left(1 - \frac{1}{M_0} \sum_{\alpha,\pi} |\langle f|a^\dagger_\alpha|\pi\rangle|^2\, \Omega^\pi_\alpha \right) \,, \end{aligned} \tag{11}$$

where $\Omega^\pi_\alpha = (1 - r^\pi_\alpha)$ is a radial-mismatch factor. With the definition of the ISB correction factor in Eq. (2), TH approximate δ_{C2} by

$$\delta_{C2} \approx \frac{2}{M_0} \sum_{\alpha,\pi} |\langle f|a^\dagger_\alpha|\pi\rangle|^2\, \Omega^\pi_\alpha \,. \tag{12}$$

Consequently, large contributions to δ_{C2} come with a large spectroscopic amplitude and a significant radial mismatch.

In evaluating δ_{C2} of Eq. (12), TH use guidance from experiment. Their results are based on shell model calculations of the spectroscopic amplitudes, but limit the sums over orbitals α and intermediate states π to those for which large spectroscopic factors have been observed in pick-up reactions. For ^{46}V, TH [6] use this strategy to include two *sd* core orbitals, $s_{1/2}$ and $d_{3/2}$, in addition to the $f_{7/2}$ orbital of their earlier calculations. Their new result for δ_{C2} is 0.58% (see Table I in Ref. [6]), which is almost a factor two larger than the 2002 value [4].

For the radial integrals, TH use the strong constraint that the asymptotic forms of all radial functions must match experimentally measured neutron and proton separation energies. In many cases, TH have to truncate the model space to keep the calculations tractable. Their final values for δ_{C2} range between 0.17 and 1.50%, and increase with mass number (see Table II in Ref. [6]).

B. Isospin-mixing correction δ_{C1}

The isospin-mixing correction δ_{C1} is obtained by setting all radial integrals to unity, but including ISB corrections to the matrix elements of the creation and annihilation operators, $\langle f|a_\alpha^\dagger|\pi\rangle^*$ and $\langle\pi|a_\alpha|i\rangle$. These arise because the neutron-rich and proton-rich states are different. TH find that calculations of δ_{C1} are very sensitive to the details of the shell-model computation, but try to reduce the model dependence by using various experimental information [6].

To obtain δ_{C1}, TH use experimental single-particle energies (on top of the core of the shell model calculation), which differ for neutrons and protons. In addition, they include a two-body Coulomb interaction among the valence protons and increase all $T = 1$ neutron-proton matrix elements (relative to the neutron-neutron ones), so that the measured b and c coefficients of the isobaric multiplet mass equation (IMME) are reproduced. Finally, TH account for weak transitions that can occur to non-analog 0^+ states. The adopted values for δ_{C1} range between 0.01 and 0.35%, and also increase with mass number (see Table III in Ref. [6]).

IV. EXACT FORMALISM AND THEOREMS FOR ISB CORRECTIONS

In this section, we present an exact formalism, independent of feasibility. We use this formalism to derive two theorems, which show that there are no first-order ISB corrections to Fermi matrix elements. This provides a perturbative expansion, which allows for a simple estimate of δ_C.

We use the correct isospin operator

$$\tau_+ = \sum_\alpha a_\alpha^\dagger b_\alpha \,, \tag{13}$$

where α represents *any* single-particle basis, and $a_\alpha^\dagger$ creates neutrons and b_α annihilates protons in state α. The Fermi matrix element is then given by

$$M_F = \langle f|\tau_+|i\rangle \,, \tag{14}$$

with $|i\rangle$ and $|f\rangle$ the exact initial and final eigenstates of the full Hamiltonian $H = H_0 + V_C$, with energy E_i and E_f, respectively. Here V_C denotes the sum of *all* interactions that do not commute with the vector isospin operator $\mathbf{T} = \sum_{i=1}^A \boldsymbol{\tau}_i/2$,

$$[H, \mathbf{T}] = [V_C, \mathbf{T}] \neq 0 \quad \text{and} \quad [H_0, \mathbf{T}] = 0 \,. \tag{15}$$

We will use round bra and ket states to denote the eigenstates of the isospin-symmetric part of the Hamiltonian, so $H_0|n) = E_n^{(0)}|n)$. Obtaining the states $|n)$ requires a solution of the A-body problem.

The full initial eigenstate $|i\rangle$ can then be written as

$$|i\rangle = \sqrt{Z_i}\left[|i) + \frac{1}{E_i - \Lambda_i H \Lambda_i}\,\Lambda_i V_c\,|i)\right], \tag{16}$$

with projector $\Lambda_i \equiv 1 - |i)(i|$, or equivalently,

$$|i\rangle = \sqrt{Z_i}\,|i) + \frac{1}{E_i - \Lambda_i H_0 \Lambda_i}\,\Lambda_i V_c\,|i\rangle \,. \tag{17}$$

Similarly, the full final eigenstate $|f\rangle$ is given by

$$|f\rangle = \sqrt{Z_f}\left[|f) + \frac{1}{E_f - \Lambda_f H \Lambda_f}\,\Lambda_f V_c\,|f)\right], \tag{18}$$

with $\Lambda_f = 1 - |f)(f|$. The factors Z_i and Z_f are taken to be real and ensure that the full eigenstates $|i\rangle$ and $|f\rangle$ are normalized. As a result, it follows (due to the projection operators) that the deviations of Z_i and Z_f from unity start at second order in V_c.

We now evaluate Eq. (14) between the exact eigenstates given by Eqs. (16) and (18). With $(f|\,\tau_+\Lambda_i = 0$ and $\Lambda_f\tau_+\,|i) = 0$, we obtain

$$M_F = \sqrt{Z_i Z_f}\left[M_0 + (f|\,V_c\Lambda_f\,\frac{1}{E_f - \Lambda_f H \Lambda_f}\,\tau_+\,\frac{1}{E_i - \Lambda_i H \Lambda_i}\,\Lambda_i V_c\,|i)\right], \tag{19}$$

where $M_0 = (f|\tau_+|i)$. Since $Z_{i,f} = 1 + \mathcal{O}(V_C^2)$, it follows that ISB contributions start at second order. This is our first theorem and demonstrates that there are no first-order ISB corrections to M_F.

We obtain a simpler form by expanding in the *difference* of the charge-dependent interactions ΔV_C between the initial proton-rich and final neutron-rich states. Hence, ΔV_C includes all charge-dependent interactions of the extra proton with the other nucleons in the initial state. In this case, we have

$$|f\rangle = |f) \quad \text{and} \quad |i\rangle = \sqrt{Z}\,|i) + \frac{1}{E_i - \Lambda_i \widetilde{H}_0 \Lambda_i}\,\Lambda_i \Delta V_C\,|i\rangle\,, \tag{20}$$

where the first expression defines ΔV_C and $\widetilde{H}_0$ includes the effects of V_C common to the initial and final states, for example the Coulomb interactions in the core.

In this case, the final state is an eigenstate of $\widetilde{H}_0$ and obeys $\langle f|\,\tau_+ \Lambda_i = 0$. As a result, it follows that

$$M_F = \sqrt{Z}\,M_0\,. \tag{21}$$

This is our second theorem. As already shown, there are no first-order ISB corrections to Fermi matrix elements, and in this case $\delta_C = 1 - Z$ has a straightforward perturbative expansion in ΔV_C, starting at second order:

$$\delta_C = (i|\,\Delta V_C \Lambda_i \left(\frac{1}{E_i - \Lambda_i \widetilde{H}_0 \Lambda_i}\right)^2 \Lambda_i \Delta V_C\,|i) + 2\mathrm{Re}\left[(i|\,\Delta V_C \Lambda_i \left(\frac{1}{E_i - \Lambda_i \widetilde{H}_0 \Lambda_i}\right)^2 \Lambda_i \Delta V_C \frac{1}{E_i - \Lambda_i \widetilde{H}_0 \Lambda_i}\,\Lambda_i \Delta V_C\,|i)\right] + \dots\,, \tag{22}$$

which follows from the normalization condition $\langle i|i\rangle = 1$. To second order in ΔV_C, the full energy E_i can be taken as the energy $\widetilde{E}_i^{(0)}$ of $\widetilde{H}_0$. Examining the third-order term of Eq. (22) [17] also shows that it is impossible to separate δ_C into two distinct terms. This is because it is not possible to distinguish whether the middle ΔV_C is part of a correction to an intermediate state $|\pi\rangle$ or to the initial state $|i\rangle$. Finally, we note that the two theorems are more general versions of the theorem of Behrends-Sirlin [13] for CVC in nucleons and of Ademollo-Gatto [14] for weak decays of kaons.

A. Simple estimate of δ_C

As an illustration of the above formalism, we calculate δ_C for the case of a single particle outside an inert core of charge Ze, assuming harmonic-oscillator single-particle wave functions with oscillator frequency $\omega \approx 39\,\mathrm{MeV}\,A^{-1/3}$. The nuclear Coulomb potential arises from the convolution of $Ze^2/(4\pi|\mathbf{r} - \mathbf{r}'|)$ with the charge density $\rho_C(r')$. If we take the latter to be a constant within $r \leqslant R$, the one-body Coulomb potential takes the simple form:

$$\Delta V_C(r) = \frac{Ze^2}{4\pi R}\left[\Theta(R-r)\left(\frac{3}{2} - \frac{r^2}{2R^2}\right) + \Theta(r-R)\,\frac{R}{r}\right] \tag{23}$$

With $R = 1.1\,\mathrm{fm}\,A^{1/3}$, we have $R\omega = 0.22$, independent of A, and therefore the correction scales as $\delta_C \sim Z^2$. To make an estimate, we take the state $|i)$ to be in the single-particle orbit with radial quantum number $n = 0$ and angular momentum l. Using Eq. (22), we find

$$\delta_C(l) = \frac{Z^2 e^4}{4(4\pi)^2 R^2 \omega^2} \sum_{n>0} \frac{1}{n^2} \left\{ \int r^2 dr\, R_{0l}(r) \left[\Theta(R-r)\left(\frac{3}{2} - \frac{r^2}{2R^2}\right) + \Theta(r-R)\,\frac{R}{r}\right] R_{nl}(r) \right\}^2 . \tag{24}$$

We calculate the summation numerically taking R equal to the oscillator length. This leads to

$$\delta_C(0) = 0.0020\%\,Z^2 \quad \delta_C(1) = 0.0013\%\,Z^2$$
$$\delta_C(2) = 0.00071\%\,Z^2 \quad \delta_C(3) = 0.00043\%\,Z^2\,. \tag{25}$$

For a $Z = 20$ core and $l = 3$, we find $\delta_C(3) = 0.17\%$ and thus $\delta_C = 3.33 \times \delta_C(3) = 0.57\%$, where the factor of 3.33 arises from the Macfarlane-French sum rule [15] for the three protons in the $f_{7/2}$ orbit. This result is in qualitative agreement with the TH contribution of 0.45% (see Table I for ^{46}V in Ref. [6]). This indicates that Eq. (21) could be a useful starting point for realistic calculations.

V. SCHEMATIC MODELS

Next we present exact evaluations of the Fermi matrix element for schematic models of increasing complexity, and compare our results to the treatment of TH.

A. One-body problem

Consider starting from the exact formalism. We can derive an effective single-particle potential $U+U_C$, where U_C accounts for charge-dependent effects and acts only on protons. The single-particle potential is introduced to minimize the effects of residual interactions

$$\Delta V = V + V_C - (U + U_C)\,. \tag{26}$$

Then the Hamiltonian is given by

$$H = T + U + U_C + \Delta V = H_{\rm sp} + \Delta V\,. \tag{27}$$

In the simplest case, we assume that the one-body Hamiltonian $H_{\rm sp}$ is dominant. Thus we take the initial and final states to consist of a single nucleon outside an inert core $|0\rangle$. The core and nucleon have quantum numbers so that the coupled state is 0^+ with $T = 1$.

The one-body basis states can be taken as eigenstates of the full single-particle Hamiltonian $T+U+U_C$, which we denote by $|\alpha\rangle$, or by the eigenstates $|\widetilde{\alpha}\rangle$ of the isospin-symmetric part $T+U$. Here U_C is the difference between the proton and neutron potentials, which corresponds to $U_C \equiv U_p - U_n + V_C$ in the TH notation. The parent and daughter states are then given by

$$|i\rangle = b^\dagger_\alpha|0\rangle \quad \text{and} \quad |f\rangle = a^\dagger_{\widetilde{\alpha}}|0\rangle\,. \tag{28}$$

It is convenient to express the isospin raising operator τ_+ in a mixed representation. The creation operators of the two bases are related by

$$a^\dagger_\alpha = \sum_{\widetilde{\alpha}} a^\dagger_{\widetilde{\alpha}}\,\langle\widetilde{\alpha}|\alpha\rangle\,, \tag{29}$$

and therefore the isospin operator of Eq. (13) reads

$$\tau_+ = \sum_{\alpha,\widetilde{\alpha}} a^\dagger_{\widetilde{\alpha}}\,\langle\widetilde{\alpha}|\alpha\rangle\,b_\alpha\,. \tag{30}$$

This equation leads to an expression for M_F that is very similar to Eq. (4) of TH with the important difference that the states α and $\widetilde{\alpha}$ need not have the same radial quantum numbers:

$$M_F/M_0 = \int r^2 dr\, R^*_{\widetilde{\alpha}}(r)\,R_\alpha(r)\,. \tag{31}$$

B. One-body problem with a single core excitation

The simplest generalization of the previous problem is to allow the core to have two states, a ground state and excited state. Then the exact eigenstate is a two component wave function, where the upper component represents the single particle plus unexcited core, and the lower component has the core in the excited state. The core excitation need not have angular momentum $J = 0$, but the coupled state is 0^+ with $T = 1$. In this case, the Hamiltonian is given as a two-by-two matrix:

$$H_0 = \begin{pmatrix} H_{\rm sp} & \Delta V \\ \Delta V & H_{\rm sp} \end{pmatrix}\,, \tag{32}$$

where the second, lower component has a higher single-particle energy than the upper component. The eigenfunctions are given by two-component "spinor" wave functions, for example for the initial state:

$$\langle\mathbf{r}|i\rangle = \begin{pmatrix} \alpha_i\,U_i(\mathbf{r}) \\ \beta_i\,L_i(\mathbf{r}) \end{pmatrix}\,, \tag{33}$$

with normalizations given by

$$\int d\mathbf{r}\,|U_i(\mathbf{r})|^2 = \int d\mathbf{r}\,|L_i(\mathbf{r})|^2 = 1 \quad \text{and} \quad \alpha_i^2 + \beta_i^2 = 1\,, \tag{34}$$

and where we have taken α, β to be real for simplicity.

The presence of the charge-dependent interaction U_C (in $H_{\rm sp}$) and of V_C (in ΔV) causes the initial and final state values of α, β and their radial wave functions to differ. In this model, the single-particle wave functions for i and f represent directly the single proton and neutron. The exact value of M_F is thus given by:

$$M_F/M_0 = \alpha_f\,\alpha_i \int d\mathbf{r}\,U^*_f(\mathbf{r})\,U_i(\mathbf{r}) + \beta_f\,\beta_i \int d\mathbf{r}\,L^*_f(\mathbf{r})\,L_i(\mathbf{r})\,, \tag{35}$$

since the core and its excitation are orthogonal. This may be rewritten as:

$$M_F/M_0 - 1 = -\alpha_i^2\,\Omega^{(1)} - \beta_i^2\,\Omega^{(2)} + (\alpha_f - \alpha_i)\,\alpha_i\,(1 - \Omega^{(1)}) + (\beta_f - \beta_i)\,\beta_i\,(1 - \Omega^{(2)})\,, \tag{36}$$

where in the TH notation

$$\Omega^{(1)} \;=\; 1 - \int d\mathbf{r}\,U^*_f(\mathbf{r})\,U_i(\mathbf{r})\,, \tag{37}$$

$$\Omega^{(2)} \;=\; 1 - \int d\mathbf{r}\,L^*_f(\mathbf{r})\,L_i(\mathbf{r})\,. \tag{38}$$

We next use the strategy of TH to evaluate this two-state core model. The states $|\pi\rangle$ consist of the ground state core and its excitation labeled by $1, 2$. For each of these, there is only one value for the single-particle index α. Therefore, the TH result for this model reads

$$M_F^{\rm TH}/M_0 - 1 \;\approx\; -\alpha_i^2\,\Omega^{(1)} - \beta_i^2\,\Omega^{(2)} + \;(\alpha_f - \alpha_i)\,\alpha_i + (\beta_f - \beta_i)\,\beta_i\,. \tag{39}$$

The contributions on the first line of Eq. (39) correspond to δ_{C2} and the terms on the second line to δ_{C1}.

In comparison with the exact result, we observe that TH neglect terms of order $(\alpha_f - \alpha_i)\Omega^{(1)}$. The relevant radial integrals are of infinite order in U_C, so that setting them to unity in evaluating the second line of Eq. (39) may be significant relative to the required accuracy, in particular if the neutron and proton separation energies are very different. In addition, this schematic model indicates that the normalization conventions of Eq. (34) are just a choice, so that the separation into the two terms δ_{C1}, δ_{C2} seems rather arbitrary. It is just as reasonable to use the product $\alpha_i U_i(\mathbf{r})$ as the upper component $\widetilde{U}_i(\mathbf{r})$ and $\beta_i L_i(\mathbf{r})$ as the lower component $\widetilde{L}_i(\mathbf{r})$ with the normalization $\int d\mathbf{r}\left(|\widetilde{U}_i(\mathbf{r})|^2+|\widetilde{L}_i(\mathbf{r})|^2\right)$. For that convention, the factors $\alpha_{i,f}, \beta_{i,f}$ would disappear from the formalism, and the separation of δ_C into δ_{C1}, δ_{C2} would neither be necessary nor possible.

1. *Evaluation using simple interactions*

Let the state $|f\rangle$ be governed by a harmonic oscillator Hamiltonian H_0,

$$H_0 = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 r^2\,, \tag{40}$$

and the state $|i\rangle$ by the Hamiltonian H, with

$$H = H_0 + V_C\,. \tag{41}$$

We use the inner form of the Coulomb potential, Eq. (23), to obtain simple expressions that show the order of various terms,

$$V_C(r) = -\frac{Ze^2}{4\pi R}\,\frac{r^2}{2R^2}\,. \tag{42}$$

This is a qualitative approximation that has been traditionally used to assess the size of various effects [11].

In this case, the Coulomb interaction shifts the square of the oscillator frequency from ω^2 to $\omega^2(1-\delta)$, where the shift δ is given by

$$\delta = \frac{Ze^2}{4\pi m\omega^2 R^3}\,. \tag{43}$$

We will consider the two lowest states with $n = 0, 1$ and angular momentum $l = 0$ to study the effects of configuration mixing.

Then for the final state single-particle basis, we have

$$(\mathbf{r}|0) \;=\; \frac{1}{(\pi b^2)^{3/4}}\,e^{-r^2/2b^2}\,, \tag{44}$$

$$(\mathbf{r}|1) \;=\; \sqrt{\frac{3}{2}}\left(1-\frac{2r^2}{3b^2}\right)\frac{1}{(\pi b^2)^{3/4}}\,e^{-r^2/2b^2}\,, \tag{45}$$

with oscillator length $b = (m\omega)^{-1/2}$. The initial state wave functions $(\mathbf{r}|\widetilde{0})$ and $(\mathbf{r}|\widetilde{1})$ have the same form, but with oscillator length

$$\widetilde{b}^2 = \frac{b^2}{1-\delta/2}\,. \tag{46}$$

With this, we find the radial overlaps:

$$(0|\widetilde{0}) \;=\; \left[\frac{1-\delta/2}{(1-\delta/4)^2}\right]^{3/4} = 1 - \frac{3\,\delta^2}{64} + \mathcal{O}(\delta^3)\,, \tag{47}$$

$$(1|\widetilde{1}) \;=\; \frac{(1-\delta/2)^{3/4}\,(1-\delta/2-3\delta^2/32)}{(1-\delta/4)^{7/2}}\,, \tag{48}$$

$$(0|\widetilde{1}) \;=\; \frac{\sqrt{3}\,\delta\,(1-\delta/2)^{3/4}}{(2-\delta/2)^{5/2}}\,, \tag{49}$$

$$(1|\widetilde{0}) \;=\; -(0|\widetilde{1})\,. \tag{50}$$

Now consider configuration mixing between the states 0 and 1 by strong interactions. As as a result, we have

$$|f\rangle \;=\; \alpha\,|0) + \beta\,|1)\,, \tag{51}$$

$$|i\rangle \;=\; \widetilde{\alpha}\,|\widetilde{0}) + \widetilde{\beta}\,|\widetilde{1})\,, \tag{52}$$

where we take $\alpha, \beta, \widetilde{\alpha}$ and $\widetilde{\beta}$ to be real for simplicity, and the quantities $\widetilde{\alpha} - \alpha$ and $\widetilde{\beta} - \beta$ are of order δ^2.

The Fermi matrix element is then given by

$$M_F/M_0 = \alpha\widetilde{\alpha}\,(0|\widetilde{0}) + \beta\widetilde{\beta}\,(1|\widetilde{1}) + [\alpha\widetilde{\beta} - \beta\widetilde{\alpha}]\,(0|\widetilde{1})\,. \tag{53}$$

The first two terms are equal to $1+\mathcal{O}(\delta^2)$. Since $\widetilde{\alpha} = \alpha + \mathcal{O}(\delta^2)$ and similarly for $\widetilde{\beta}$, the leading first-order part of $(0|\widetilde{1})$ (see Eq. (49)) thus cancels exactly, and the last two terms of Eq. (53) start at order δ^3. This validates that there are no first-order ISB corrections to M_F, and shows that certain approximations can violate our theorems.

C. Two interacting nucleons outside an inert core

Next we assume an inert core and two interacting nucleons with total angular momentum $J = 0$. The initial state wave function can have components spread over different single-particle configurations with radial, orbital and total quantum numbers n, l, j:

$$|i\rangle = \sum_{n_1,n_2,l,j,m} \langle j, m, j, -m|0, 0\rangle \times A_i^{n_1,n_2,l,j}\, b^\dagger_{n_1 lj,m}\, b^\dagger_{n_2 lj,-m}\,|0\rangle\,. \tag{54}$$

For clarity, we have taken two protons $(b^\dagger)^2$ on top of a 0^+ core, coupled to $J = 0$, $M_J = 0$. A similar expression for the final state involves the amplitudes $A_f^{n_1,n_2,l,j}$, which differ due to the effects of the charge-dependent

interactions. In this way, two-nucleon correlations are incorporated in a limiting case of the formalism of Sect. IV.

The exact expression for M_F is then given by

$$M_F/M_0 = \sum_{n_1,n_1',n_2,l,j} A_f^{n_1,n_2,l,j\,*}\, A_i^{n_1',n_2,l,j} \times \int r^2 dr\, R_f^{n_1' l\,*}(r) R_i^{n_1 l}(r)\,, \quad (55)$$

with radial wave functions $R_{i,f}$. For example, n_1 could correspond to states in the shell-model valence space and n_1' to a high-lying shell due to strong interactions.

The TH approximation for M_F would be

$$M_F^{\rm TH}/M_0 \approx \sum_{n_1,n_2,l,j}^{\text{model space}} \Big[|A_i^{n_1,n_2,l,j}|^2 \left(1-\Omega^{(n_1 l j)}\right) + \left(A_f^{n_1,n_2,l,j\,*} - A_i^{n_1,n_2,l,j\,*}\right) A_i^{n_1,n_2,l,j} \Big]. \quad (56)$$

We compare the exact result of Eq. (55) with the TH approximation Eq. (56):

1. We find corrections to the radial overlaps, because the quantum numbers n_1 and n_1' need not be equal.

2. The exact result mixes in higher-lying configurations that are not within the TH model space. To incorporate ISB effects due to higher-lying states, one needs to evaluate their contributions to charge-dependent effective interactions. In particular, an interesting topic for future study is the renormalization from long-range Coulomb effects.

3. As in the previous models, the radial integrals of Eq. (55) are of infinite order in V_C, so that setting them to unity in evaluating δ_{C2} might not be very accurate.

D. Two nucleons with a single core excitation

This model combines those of the two previous subsections. The core can be excited so that the two interacting nucleons are outside a core in its ground or excited state. Using the previously adopted notation, the exact value of M_F reads

$$M_F/M_0 = \sum_{n_1,n_1',n_2,l,j} \times \Big[A_f^{n_1,n_2,l,j\,*} A_i^{n_1',n_2,l,j} \int r^2 dr\, U_f^{n_1' l\,*}(r) U_i^{n_1 l}(r) + B_f^{n_1,n_2,l,j\,*} B_i^{n_1',n_2,l,j} \int r^2 dr\, L_f^{n_1' l\,*}(r) L_i^{n_1 l}(r) \Big], \quad (57)$$

and the TH approximation would be

$$M_F^{\rm TH}/M_0 \approx \sum_{n_1,n_2,l,j}^{\text{model space}} \Big[|A_i^{n_1,n_2,l,j}|^2 \left(1-\Omega_1^{(n_1 l j)}\right) + \left(A_f^{n_1,n_2,l,j\,*} - A_i^{n_1,n_2,l,j\,*}\right) A_i^{n_1,n_2,l,j} + |B_i^{n_1,n_2,l,j}|^2 \left(1-\Omega_2^{(n_1 l j)}\right) + \left(B_f^{n_1,n_2,l,j\,*} - B_i^{n_1,n_2,l,j\,*}\right) B_i^{n_1,n_2,l,j} \Big]. \quad (58)$$

VI. CONCLUSIONS

We have studied the formalism to include ISB corrections to Fermi matrix elements, motivated by the recent experimental achievements on $0^+ \to 0^+$ nuclear β decay and by the work of Towner and Hardy [6]. This is a key challenge for nuclear theory and pivotal for extracting the up-down CKM matrix element, which provides precision tests of the Standard Model.

We have shown that TH do not use the isospin operator of the Standard Model to calculate ISB corrections. It is also true that their separation $\delta_C = \delta_{C1} + \delta_{C2}$ is model dependent [4]. Using a complete formalism, we derived two theorems, which demonstrate there are no first-order ISB corrections to Fermi matrix elements.

Towner and Hardy correctly include the leading part of the Coulomb effects on the radial wave functions. We have found corrections to the TH treatment, and contrasted these to exact results in schematic models of increasing complexity. One of the differences is that the radial overlaps need not have the same radial quantum numbers (as assumed in TH). This mixing has also been pointed out in density-functional based calculations of ISB corrections [16]. In addition, significant to the required accuracy, there may be contributions from higher-lying configurations that are outside the model space. This requires a careful inclusion into charge-dependent effective interactions, where our accurate understanding of isospin-symmetry breaking in nuclear forces can be very helpful, and a careful study of truncation effects, where modern methods can lead to improvements.

Numerical evaluations using the formalism presented here are needed as a next step. We hope that our work stimulates further efforts to make systematic improvements to the important problem of ISB corrections to superallowed transitions.

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